

Propanamide, 2-hydroxy-2-methyl-
13027-88-8 | DTXSID8065327

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.66 days

Global applicability domain: Outside

Local applicability domain index: 3.63e-01

Confidence level: 7.47e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene

Measured: 24.3

Predicted: 4.02

Image not found

Ethylbenzene

Measured: 120

Predicted: 6.21

Image not found

Ethylcyclopentane

Measured: 511

Predicted: 8.14

Image not found

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95

Image not found

1,3-Diethylbenzene

Measured: 88.3

Predicted: 5.36